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MODELING DISLOCATIONS AND DISCLINATIONS WITH FINITE MICROPOLAR ELASTOPLASTICITY

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ABSTRACT Presented are aspects of a constitutive model for crystalline metals containing dislocation and disclination defects. Kinematics and balance laws are developed simultaneously at two scales of observation. The macroscopic kinematic description is characterized by a multiplicative decomposition of the deformation gradient, while the meso-level description follows from an additive decomposition of a connection into objects reflecting dislocations and disclinations. At the macroscale, the standard linear and angular momentum balances are enforced, while at the mesoscale, we postulate additional momentum equations for driving forces conjugate to defect densities.

INTRODUCTION Experiments have indicated the formation of misoriented rotational and/or laminar defect substructures within grains of ductile metals subjected to large deformations [cf. Ortiz & Repetto, 1999]. Following previous generalized continuum theories of crystal defects [Minagawa, 1979; Peçherski, 1983; Bammann, 2001], we develop a finite strain micropolar model wherein continuously distributed dislocations and disclinations capture the physics of evolving defect patterns at multiple length scales.

PROCEDURES, RESULTS, AND DISCUSSION The deformation gradient $F^a_{.A}$ is decomposed multiplicatively as

$$F^a_{.A} \equiv \partial x^a / \partial X^A = F^{ea}_{.\alpha} \hat{R}^\alpha_{.\bar{A}} F^{p\bar{A}}_{.A} \qquad (1)$$

where Cartesian current coordinates $x^a = \phi^a(X^A, t)$, and where $F^{ea}_{.\alpha}$, $\hat{R}^\alpha_{.\bar{A}}$, and $F^{p\bar{A}}_{.A}$ are the elastic deformation, the lattice rotation due to the time history of disclination flux, and the plastic deformation attributed to the time history of dislocation flux. We can further decompose the elastic deformation into compatible and incompatible parts:

$$F^{ea}_{.\alpha} = F^{ca}_{.\tilde{a}} F^{i\tilde{a}}_{.\alpha}, \qquad 2F^{c-1\tilde{a}}_{.[a,b]} \equiv F^{c-1\tilde{a}}_{.a,b} - F^{c-1\tilde{a}}_{.b,a} = 0, \qquad (2)$$

with the subscripted comma denoting partial coordinate differentiation. Disclinations are assumed to only induce rotation, i.e., $\hat{R}^{T\bar{A}}_{.\alpha} = \hat{R}^{-1\bar{A}}_{.\alpha}$ [Lardner, 1973; Peçherski, 1983]. We next introduce linear connection coefficients Γ^a_{bc} and the rank two metric tensor C^e_{ab}:

$$\Gamma^a_{bc} \equiv F^{e\,a}_{.\alpha} F^{e-1\,\alpha}_{.c,b} + Q^a_{bc}, \qquad C^e_{\;ab} \equiv F^{e-1\,\alpha}_{.a} \delta_{\alpha\beta} F^{e-1\beta}_{.b}, \qquad (3)$$

with $F^{e\,a}_{.\alpha} F^{e-1\,\alpha}_{.c,b}$ the so-called "crystal connection" of non-Riemannian dislocation theories, and with Q^a_{bc} a micropolar rotation mode associated with disclinations [Minagawa, 1979], subject to the anti-symmetry requirements $Q_{bca} \equiv Q^d_{bc} C^e_{\;da} = Q_{b[ca]}$. The torsion and curvature, respectively, of Γ^a_{bc} are written as [Schouten, 1954]

$$T^a_{bc} = F^{e\,a}_{.\alpha}(F^{I-1\,\alpha}_{.\beta,b} F^{e-1\beta}_{.c} - F^{I-1\,\alpha}_{.\beta,c} F^{e-1\beta}_{.b}) + 2Q^a_{[bc]}, \quad R_{abcd} = R_{[ab][cd]} = 2\nabla_{[c} Q_{d][ba]} + T^e_{cd} Q_{e[ba]}, \quad (4)$$

where ∇_a denotes covariant differentiation with respect to Γ^a_{bc}. The dislocation density α^{ab} and the disclination density θ^{ab}, both referred to the spatial frame, are then found as

$$2\alpha^{ab} \equiv \varepsilon^{bcd} T^a_{cd}, \qquad 4\theta^{ef} \equiv \varepsilon^{eba} \varepsilon^{fcd} R_{abcd}. \qquad (5)$$

Using Schouten's [1954] identity $R_{a[bcd]} = T_{a[bc,d]}$ and Bianchi's equations $R_{ab[cd,e]} = 0$, conservation laws for the defect densities are written as [Minagawa, 1979]

$$C^e_{\;ab} \alpha^{bc}_{..c} + \varepsilon_{abc} \theta^{bc} = 0, \qquad \theta^{ab}_{..b} = 0. \qquad (6)$$

We assume a general free energy potential, per unit mass, with the functional dependency

$$\psi = \psi(\bar{C}^e_{\;\alpha\beta}, \alpha^{ab}, \theta^{ab}, \varepsilon), \qquad (7)$$

where $\bar{C}^e_{\;\alpha\beta} \equiv F^{e\,a}_{.\alpha} g_{ab} F^{e\,b}_{.\beta}$ (with the Euclidean spatial metric g_{ab}) and where $\varepsilon = b\sqrt{\rho_s}$ is a dimensionless measure of the statistically-stored dislocation line length per unit current volume ρ_s, with b the magnitude of the Burgers vector. The local energy balance and entropy inequality, under strictly isothermal conditions, are written, respectively, as

$$(1/2)\sigma^{ab}(\mathcal{L}_v g)_{ba} + \chi_{ab}\dot{\alpha}^{ab} + \xi_{ab}\dot{\theta}^{ab} = \rho\dot{e} \geq \rho\dot{\psi}, \qquad (8)$$

with ρ the current mass density, e the internal energy, σ^{ab} the symmetric Cauchy stress satisfying $\sigma^{ab}_{..b} + \rho f^a = \rho\dot{v}^a$, χ_{ab} and ξ_{ab} generalized meso-level stresses, and $\mathcal{L}_v$ the Lie derivative with respect to the velocity field $v^a \equiv \dot{x}^a \circ \phi^{-1}_t$. Substituting (7) into (8)$_2$ gives

$$\sigma^{ab} = 2\rho(\partial\psi / \partial g_{ab}), \qquad \sigma^{ab} g_{bc} F^{ec}_{.\alpha} \dot{\hat{F}}^{\alpha}_{.A} \hat{F}^{-1A}_{.\beta} F^{e-1\beta}_{.a} - \kappa\dot{\varepsilon} \geq 0, \qquad (9)$$

where we define $\hat{F}^{\alpha}_{.A} \equiv \hat{R}^{\alpha}_{.A} F^{p}_{.A}$ and $\kappa \equiv \rho\partial\psi/\partial\varepsilon$, and also provides the conjugate thermodynamic force relations $\chi_{ab} = \rho\partial\psi/\partial\alpha^{ab}$ and $\xi_{ab} = \rho\partial\psi/\partial\theta^{ab}$. We now make the more specific assumption

$$\rho\psi = \rho\psi_1(\bar{C}^e_{\;\alpha\beta}) + (1/2)\mu(l_\alpha^2 \alpha^{ab} g_{ac} g_{bd} \alpha^{cd} + l_\theta^4 \theta^{ab} g_{ac} g_{bd} \theta^{cd} + c\varepsilon^2), \qquad (10)$$

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with ψ_1 the recoverable energy and μ, l_α, l_θ, and c an elastic shear modulus, length parameter associated with dislocations, length parameter associated with disclinations, and dimensionless scalar. Quasi-static mesoscopic momentum balances are postulated as [Bammann, 2001]

$$g^{cb}\chi_{ac,b} = 0, \qquad\qquad g^{cb}\xi_{ac,b} + g_{ad}\varepsilon^{dbc}\chi_{bc} = 0. \tag{11}$$

To complete the kinetic description, expressions for the defect density fluxes are needed:

$$\dot{F}^{p\,\overline{A}}_{\ \ .A} = \dot{F}^{p\,\overline{A}}_{\ \ .A}\big(\{A^p\}\big), \quad \dot{\hat{R}}^\alpha_{.\overline{A}} = \dot{\hat{R}}^\alpha_{.\overline{A}}\big(\{A^r\}\big), \quad \dot{Q}^a_{bc} = \dot{Q}^a_{bc}\big(\{A^q\}\big), \quad \dot{\varepsilon} = \dot{\varepsilon}\big(\{A^\varepsilon\}\big), \tag{12}$$

where $\{A^p\}$, $\{A^r\}$, $\{A^q\}$, and $\{A^\varepsilon\}$ denote tensor functions of the appropriate rank depending explicitly upon the members of the set $\big(\sigma^{ab}, \chi_{ab}, \xi_{ab}, \kappa, \chi_{ab,c}\big)$ mapped to suitable configurations. Spatial gradients of the dislocation density reflecting the contribution of pile-ups to hardening are embodied by the term $\chi_{ab,c}$. Specific forms of (12) must be developed, subject to constraints imposed by inequality (9)$_2$ and the force balances (11). As an alternative to (12)$_2$, $\hat{R}^\alpha_{.\overline{A}}$ can be found explicitly in terms of θ^{ab} assuming stationary disclinations [Lardner, 1973]. If we further assume that Q^a_{bc} satisfies the integrability conditions $Q^a_{bc} = q^a_{.bc} = Q^a_{cb}$, then the six equations in (11) are sufficient to determine the six independent components of Q^a_{bc} and (12)$_3$ is not needed. Characteristic defect patterns are expected to emerge as a result of certain prescriptions of l_α, l_θ, c, and Eqs. (12) leading to non-convexity of the energy potential (10) [Ortiz & Repetto, 1999].

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